Entropy, Irreversibility and Probability in chaotic systems

Irreversibility became central to thermodynamics after Carnot's theorem determining the maximum efficiency η_{max} of a thermic machine: and η_{max} could not be reached as it had to work *reversibly*, hence infinitely slow.[1]

Carnot's theorem (1824) led Clausius (1850-1865) to introduce entropy and to formulate the II principle of Therm. relying on Carnot's theorem, which implied the possibility of defining entropy variation between equilibrium states A and B.[2, 3, 4].

Just construct a reversible transf. from A to B and add up the amounts of heat absorbed from external reservoirs divided by the respective absolute temperature, that by the time had been identified with the system average kinetic energy. [5]:

$$S(B) - S(A) = \sum \frac{Q_i}{T_i}$$

Atomists immediately asked for the mechanical meaning of entropy. Boltzmann (1866) proposed a probabilistic interpretation: observables, in equilibrium, have values which are actually averages of (often rapidly) changing instantaneous values.

Therefore an equil. state can be identified with the average values of the observables.

His first hypotesis supposed that the microscopic motion is periodic: and an equilibrium state could be identified with a single periodic trajectory. The averages would simply be deduced via the fraction of time spent in a segment of the periodic trajectory, viewed as a closed path in phase space (*i.e.* space points $\equiv$ set of molecules coordinates).

The assumption might seem surprising, but B. shewed that a well known mechanical property, namely the principle of least action, implied that the action

$$S(A) = \oint_A \vec{p} \cdot d\vec{q}$$

of the periodic trajectory had variations between A and B independent of the transformation, provided it took place so slowly that at every time it could be considered periodic.

The function S was identified with the entropy because interpreting average kinetic energy as temperature and calling dL the average work reversibly performed by the external forces it followed that the variation of the internal energy dU had the thermodynamic property

$$\frac{dU + dL}{T} = dS$$

thus justifying the interpretation as Clausius' entropy.

By 1868 he had completely founded modern Statistical Mechanics and introduced the *microcanonical ensemble*. Periodicity had become the ergodic hypothesis.
Periodic microscopic motions were replaced by a probability distribution (1868) describing an equil. state in the form

$$\rho(\vec{p},\vec{q})d\vec{p}d\vec{q}$$

and "therefore" in a motion going close to all phase space points (*i.e.* being dense) ρ had to be *positive and invariant*: hence a function of the energy H.
B. did not think about the possibility that other constants of motion exist (aside obvious exceptions) and may be not smooth: and existence of only one smooth const. of motion is the modern definition of ergodicity of a mech. system with conservative forces.

B. tried to illustrate this point by giving an example.

Probably continuing to think so, he proceeded to show that the same system could be described by very different probability distributions provided contained in a large volume V and the interesting observables depended on the particles in a region $\Lambda \subset V$ much smaller (*local observables*).

Is it possible to carry the program of B. to nonequilibrium phenomena? What about friction and irreversibility?

The first difficulty, even restricting attention to stationary states, is that in non equilibrium there are external forces which perform work generating heat and heat has to be removed. So dissipation is present.

In the equations of motion $\dot{x}_i = f_i(x)$ dissipation appears because, Liouville's theorem, a volume element dx evolves in time dt into a volume element $dx' = (1 + div \cdot dt)dx$ with $div = \sum_i \frac{\partial f_i(x)}{\partial x_i}$ and typically $div < 0$ and $dx' < dx$.

For instance in the incompressible Navier-Stokes eq., for simplicity in container with periodic b.c. $[0,2\pi]^d$, $d=2,3$, velocity is $\mathbf{u}(\mathbf{x})$ represented via Fourier's transf.

$$\mathbf{u}(\mathbf{x})=\sum_{\mathbf{k}\neq\mathbf{0}}\mathbf{u}_{\mathbf{k}}e^{2\pi\, i\,\mathbf{k}\cdot\mathbf{x}},\quad \mathbf{u}_{\mathbf{k}}\cdot\mathbf{k}=0$$

If ($\mathcal{P}_{\mathbf{k}}$= proj. on plane orth. to $\mathbf{k}$), NS equation is :

$$\dot{\mathbf{u}}_{\mathbf{k}}=-i\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}}(\mathbf{u}_{\mathbf{k}_1}\cdot\mathbf{k}_2)\mathcal{P}_{\mathbf{k}}\mathbf{u}_{\mathbf{k}_2}-\nu\mathbf{k}^2\mathbf{u}_{\mathbf{k}}+f_{\mathbf{k}}=Q_{\mathbf{k}}(\mathbf{u})-\nu\mathbf{k}^2\mathbf{u}_{\mathbf{k}}+f_{\mathbf{k}}$$

and the divergence is $div=-\nu\sum_{\mathbf{k}}\mathbf{k}^2<0$.

Actually $div=-\infty$ and, for this reason, the eq will be "regularized" by restricting all $\mathbf{k}$'s to be $|\mathbf{k}|<N$, turning Q into Q^N **and** the problem into studying properties of the reg. solutions which become N-indep. as $N\to\infty$.

Phase space contraction, always accompanying dissipation, implies that probabilities describing stationary states must be concentrated on sets of 0-volume: hence averages cannot be expressd by volume integrals.

So the basic B.'s assumption that averages of observables O could be expressed via integrals $\int O(\vec{p},\vec{q})\rho(\vec{p},\vec{q})d\vec{p}d\vec{q}$ cannot be accepted, at least not for all O, in nonequilibrium.

New idea has been that in Physics systems are studied following evolution of samples generated by some "protocol". The procedure, even if carefully built is subject to unknown influences so that the probability distrib P_0 of the data produced is unknown.

It has been proposed that it be $P_0 = \rho_0(\vec{p},\vec{q})d\vec{p}d\vec{q}$ with ρ_0 **continuous but unknown**.

This is a very strong assumption (although some may consider it not an assumption at all).

Surprisingly, in systems with chaotic evolution, it allows the unique identification of the invariant probability distribution **P** for averages of the observables. [6, 7].

It is **only** necessary to interpret chaotic evolution in terms of the paradigm offered, in the elementary dynamical systems theory for Chaos, by the hyperbolic dynamical systems $x \to S_t x$.

In such systems following the motion of a point x in phase space one sees it as a fixed point which is hyperbolic.

Thus the B. paradigm, identifying periodic motion as the "key", is replaced by the (equally "disturbing") paradigm identifying chaotic systems with hyperbolic systems.

The main point is that hyperbolic systems are very well understood, just as the dynamics of harmonic motions is.

In B.'s case periodic motion assumption was likely to be (in general) mathematically false and yet it generated Stat. Mech., likewise the hyperbolicity may be false in most cases of interest: but just like the periodicity or quasi periodicity is a paradigm for the ordered motion, so hyperbolic systems are the paradigm of chaotic motions.

Hyperbolicity hypothesis opens the way to deriving quite a few physically relevant consequences.

Among B.'s equilibrium results is that the same system can be described by completely different probability dist. on phase space: which nevertheless attribute the **same average** values to **local** observables, *i.e.* depending on particles located in volumes $\ll$ than the container vol. V.

E.g. investigate again the question of compatibility between microscopic reversibility and macroscopic irreversibility.
Start remarking that reversibility being a fundamental symmetry cannot be lost.

To be concrete consider an incompressible fluid, and to further simplify, imagine it in a periodic container $[0, 2\pi]^d$, $d = 2, 3$ and subject to a simple "large scale" stirring force $\mathbf{f}$. The NS equation is again, $\mathbf{k} \cdot \mathbf{u_k} = \mathbf{0}$ and

$$\dot{\mathbf{u}}_\mathbf{k} = Q^N(\mathbf{u})_\mathbf{k} - \nu \mathbf{k}^2 \mathbf{u}_\mathbf{k} + f_\mathbf{k}$$

and the flow $t \to S_t\mathbf{u}$ is irreversible: the temperature variable $T(x)$ is absent and the density is constant, which physically means that a thermostat acts on the system taking away the heat generated by the stirring.

It is phenomenologically represented by the viscosity term $-\nu \mathbf{k}^2 \mathbf{u}_\mathbf{k}$ and the stationary states of the fluid are a family $\mathcal{P}^{irr}$ of probability distributions $\mathbf{P}_\nu^N$ on the velocity fields, parameterized by the viscosity ν.

However viscosity, being phenomenological, can be replaced by other ways of thermostating the fluid: for instance instead of adding to the Euler equations the viscous force $-\nu \mathbf{k}^2 \mathbf{u}_\mathbf{k}$ to avoid blow up, one could add to Euler eq. a force which keeps exacly constant the "enstrophy"

$$E(\mathbf{u}) = \sum_\mathbf{k} \mathbf{k}^2 |\mathbf{u}_\mathbf{k}|^2.$$

This is a non-holonomic constraint that can be generated, **for instance**, by a force determined by Gauss' least effort principle: which here amounts to replacing

$$-\nu \mathbf{k^2} \mathbf{u}_\mathbf{k} \;\Rightarrow\; -\alpha(\mathbf{u}) \mathbf{k^2} \mathbf{u}_\mathbf{k}$$

From the new viewpoint one physical system on which a thermostat acts is governed by two equations

$$\dot{\mathbf{u}}_{\mathbf{k}} = Q(\mathbf{u})^N_{\mathbf{k}} - \begin{cases} \nu\ \mathbf{k}^2\mathbf{u}_{\mathbf{k}} \\ \alpha(\mathbf{u})\mathbf{k}^2\mathbf{u}_{\mathbf{k}} \end{cases} + f_{\mathbf{k}}$$

An elementary application of Gauss' p. yields in $d = 2$

$$\alpha(\mathbf{u}) = \frac{\sum_{\mathbf{k}} \mathbf{k}^2 \mathbf{f}_{-\mathbf{k}} \cdot \mathbf{u}_{\mathbf{k}}}{\sum_{\mathbf{k}} \mathbf{k}^4 |\mathbf{u}_{\mathbf{k}}|^2}$$

Imposing that the stirring does not heat the incompressible fluid can be achieved either by a phenom. friction force or by a force keeping $\mathcal{D}(\mathbf{u}) = \sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{u}_{\mathbf{k}}|^2$ constant, which amounts to a variable friction. *I.e.* friction is not fundamental.

Of course one can envisage other ways to balance stirring and heating. For instance the Enstrophy constraint could be replaced by the constraint of constant Energy.

If this is correct we have two equations for the same system: only possibility is their equivalence.

Remark that while the first flow, $t \to S_t^{irr}\mathbf{u}$ is irreversible, *i.e.* the time reversal symmetry $I\mathbf{u} = -\mathbf{u}$ is such that $IS_t^{irr} \neq S_{-t}^{irr}I$, the second is reversible because $\alpha(\mathbf{u})$ is odd: $IS_t^{rev} \equiv S_{-t}^{rev}I$

Hence the stationary states of the fluid will be described by two collection of stationary prob. distr. Context suggests strong analogy with equil. Stat. Mech.:

- **a cut-off** N: analog to container volume V of a gas.
- **a parameter** ν, which parameterizes the stationary distrib. $\mathbf{P}_\nu^{irr,N}$ of the irreversible equation analogous to the parameter β in the canonical ensemble
- **a parameter** E which parameterizes the stationary distrib. $\widetilde{\mathbf{P}}_E^{rev,N}$ of the reversible equation analogous to the parameter E in the microcanonical ensemble

To check the possibility that the same system could be described by different equations it remains to identify the class of observables with equal averages in corresponding ensembles and the correspondence $E \longleftrightarrow \nu$:

- **observables** will be $O(\mathbf{u})$ which depend on finitely many Fourier comp. $\mathbf{u_k}$: analogous to the observables depending on the partices in a finite subvolume $\Lambda \subset V$
- **corresponndence** is established by the relation

$$\mathbf{P}_\nu^{irr,N}\Big(\sum_{\mathbf{k}} \mathbf{k}^2|\mathbf{u_k}|^2\Big) = E \qquad *$$

Then the **precise conjecture** is: $*$ implies

$$\lim_{N\to\infty} \mathbf{P}_\nu^{irr,N}(O) = \lim_{N\to\infty} \widetilde{\mathbf{P}}_E^{rev,N}(O)$$

This means that in a fluid, dissipation can be modeled
1) either via a viscosity force:

$$\dot{\mathbf{u}}_{\mathbf{k}} = -Q(\mathbf{u})_{\mathbf{k}} - \nu \mathbf{k}^2 \mathbf{u}_{\mathbf{k}} + \mathbf{f}_{\mathbf{k}}$$

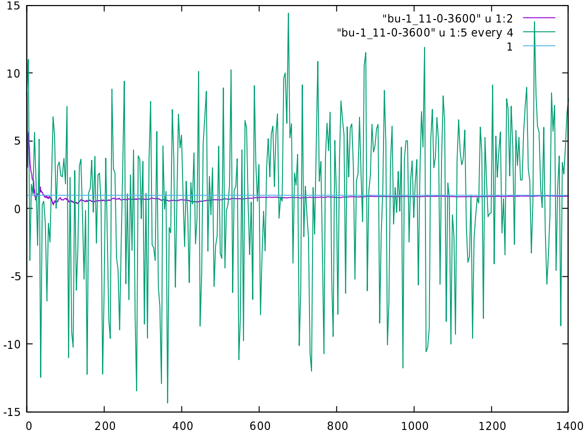
2) or requiring the enstrophy $\mathcal{D}(\mathbf{u})$ to remain constant

$$\dot{\mathbf{u}}_{\mathbf{k}} = -Q(\mathbf{u})_{\mathbf{k}} - \alpha(\mathbf{u}) \mathbf{k}^2 \mathbf{u}_{\mathbf{k}} + \mathbf{f}_{\mathbf{k}}$$

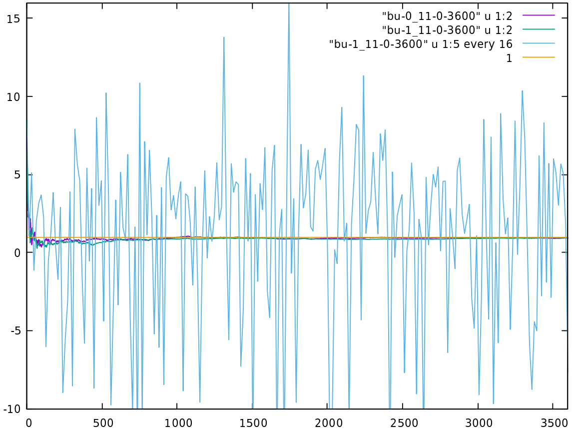
The conjecture is being tested and the results of the first few tests ar repoted in the following graphs.
1) tests began from a **rigorous consequence**

$$\widetilde{\mathbf{P}}_E^{rev,N}(\alpha) = \nu$$

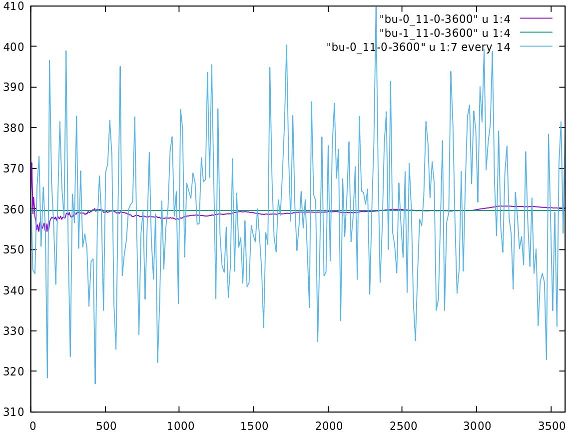
showing conjecture to be about a *homogeneization problem*.
2) Then one can take a special Fourier's component, like $\mathrm{Re}\, \mathbf{u}_{2,2}$ and study its average in the two evolutions.
3) extending the conjecture: Lyapunov spectrum of two corresponfing distr. can be studied



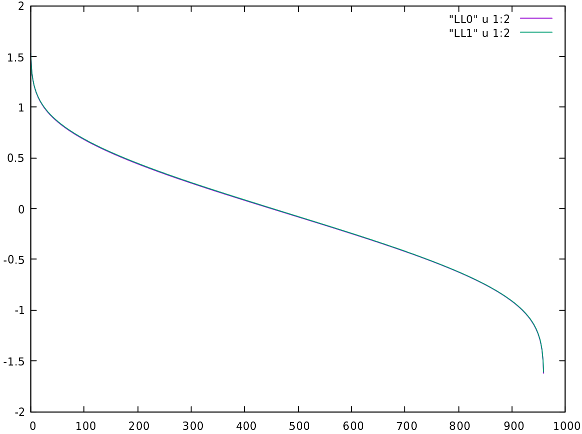
Test of running average of $\nu^{-1}\alpha(\mathbf{u}(t))$ tends to 1: reversible
x-axis= time (unit $\sim \lambda_{max}^{-1}$, step $h = 2^{-17} \sim \frac{1}{4}\lambda_{max}^{-1}$)
$N = 15$, $\mathcal{N} = 960$-Fourier's components $\mathbf{u_k}$
brown line = running average of the green$\nu^{-1}\alpha(\mathbf{u}(t)$
blue= line 1



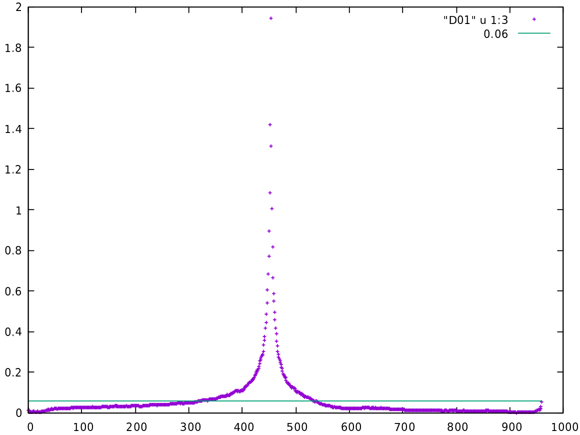
Same reversible: evolution over longer time



Irreversible evolution: running average of Enstrophy brown and the equivalent Enstrophy in the reversible evol. straight line blue fluctuating Enstrophy blue



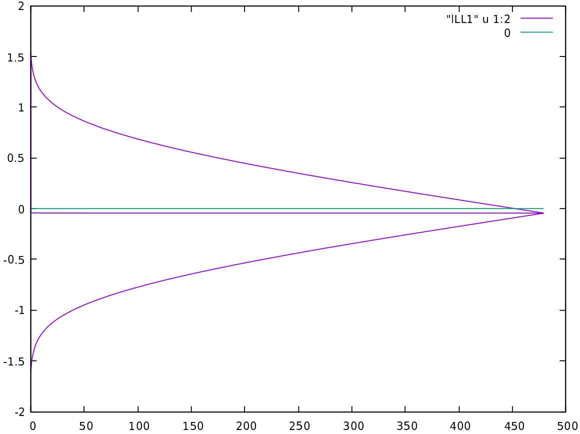
Reversible and irreversible local Lyapunov spectra (960 modes, ...)
the lines consist of $\mathcal{N} = 960$ data and look superposed



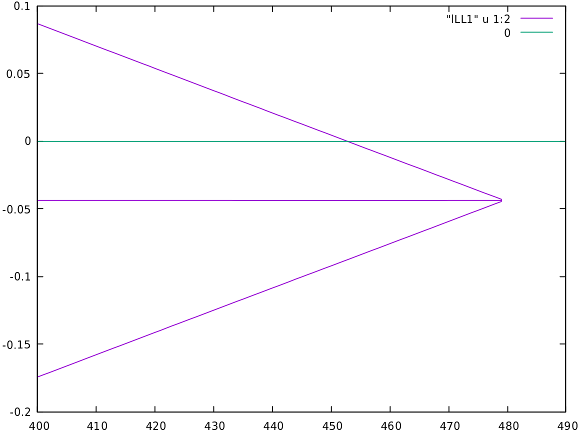
Relative difference of the previous graph:

$$k \to \frac{|\lambda_k^{rev} - \lambda_k^{irr}|}{\max(|\lambda_k^{rev}|, |\lambda_k^{irr}|)}$$

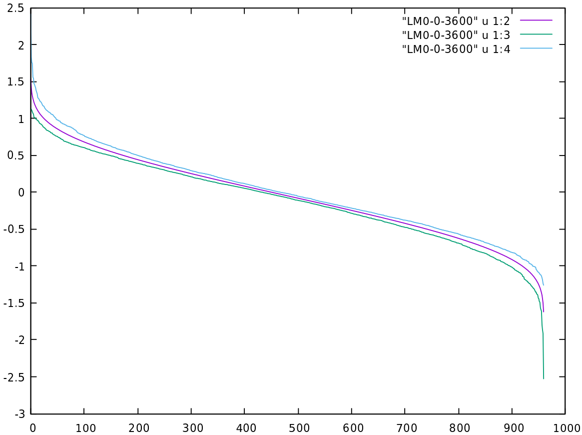
The line marks **6%**.



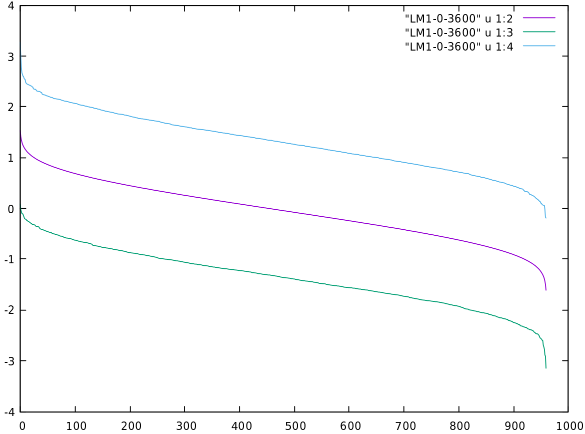
Lyapunov exp. of the previous drawing, $\mathcal{N} = 960$ drawn differently(first $\frac{1}{2}\mathcal{N}$ λ_k's followed by the next as $\lambda_{\mathcal{N}-1-k}$ $k \to \frac{1}{2}(\lambda_k + \lambda_{\mathcal{N}-1-k})$ violet (looks straight but is not)
This illustrates the (approximate) pairing rule (irreversible evol: but reversible gives same graph).



Detail: illustrates presence of a fraction of pairs < 0: interpretation (tentative): exponents relative to the approach to the attractor. If so the Kaplan Yorke fractal dimension should discard them from the count.



Irreversible exponents: the violet line is the above irreversible spectrum, equal to the reversible. The other two lines are the envelops of the maximal and minimal values averaging to the central line (*i.e.* "error estimate")



Reversible exponents: the violet line is the above reversible spectrum apparently equal to the irreversible one. The other two lines are the envelop of the maximal and minimal values averaging to the central line (*i.e.* "error estimate"). Very strong fluctuations but coinciding averages

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